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## IONIZING RADIATION EFFECTS ON TlFeS<sub>2</sub> CRYSTAL

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**Abstract:** Herein, the radiation resistance and radiation defects formation of chain semiconductor antiferromagnetic TlFeS<sub>2</sub> monocrystal irradiated with heavy ions at different doses have been investigated. It has been studied the influence of radiation with heavy xenon ions on the structure of the irradiated layer and shown that, as the radiation dose increases, the number of peaks of periodicity of the atomic clusters of nanosize surface decreases exponentially.

**Keywords:** ionizing radiation, implantation, radiation defects, surface morphology

### 1. Introduction

Development of modern science and technology requires aggressive environment - high temperature, pressure and radiation - resistant materials and devices. Since the devices sent to the space during the research of the cosmic space are under the influence of high radiation for a long time, there occur various changes in the properties of the used materials, which undermine the accuracy of the results. It is extremely urgent to study the radiation-induced defects in semiconductor materials, which form the basis of modern electronics, and as well as to study the effects of different type radiation in the most sensitive components for ensuring that this technology can be improved and controlled effectively [1,2]. Ionizing radiation is used in the investigation of the nature of radiation-induced defects, in the change of electrophysical properties of substances, in the study of surface physics, and in the protection of the material surface from the corrosion. Approximately 85% of cosmic radiation is protons, the smallest ions. Therefore in recent years, the interest in the study of the changes in the radiation resistance, the radiation effect on electrophysical properties, the interaction of the ion with the substance at the end of the running distance and the other properties of semiconductors, which are the main component of the spacecraft, caused by ionizing radiation has increased significantly [3, 4, 5, 6].

Scientists are looking for new materials, due to the increased demand of the materials that do not lose their ability to operate in a high radiation condition in space and nuclear technology, in reactors and accelerators, in space rockets, in the preparation of detector systems etc. [7-8]. The lack of radiation-resistant materials creates obstacles for the implementation of mega projects.

Layered-chain antiferromagnetic semiconductor TlMeX<sub>2</sub> (Me - 3d metal, X - S, Se, Te) type general chemical compounds, which are the most promising materials used in detector systems, electronics, phototransistors, memory elements and other objects, are of particular importance. It is important to study the changes in physical properties of TlFeS<sub>2</sub>, TlFeSe<sub>2</sub> crystals from this family in high radiation conditions. For this purpose, it is required to study extensively the influence of different type gamma rays, neutrons, electrons, protons, alpha particles, light and heavy ions, etc. on these materials. In this study, high-energy heavy ions have been selected. The main advantages of a heavy ion use in ionizing radiation are:

- creation of high-speed point defects
- relatively larger running distance

- large volume irradiation
- uneven distribution of radiation defects along the path of particles
- no activation of the sample
- control of high intensity and temperature
- obtaining high doses.

In the recent studies [8, 9], it has been shown that point defects, interatomic vacancies, increase in intercrystallite distance, the formation of clusters and generation of micro-cracks occur in these materials during the irradiation with neutrons with the energy more than 0.1 MeV and with heavy ions. As well, it is of great interest to investigate the diffusion occurrences and the mechanism of oxidation on the surface during the irradiation with low energy ions [10, 11]. At present, one of the major issues in radiation material science is the study of the mechanism of oxidation on the surface after ionizing radiation.

## 2. Experiment and measurements

For the complex structural change and the formation of radiation defects, the TlFeS<sub>2</sub> sample has been irradiated with 167 MeV energy xenon ions at  $0.5 \cdot 10^{13}$ ,  $1.0 \cdot 10^{13}$ ,  $2.0 \cdot 10^{13}$  ion/cm<sup>2</sup> radiation doses, under high dose vacuum ( $< 7 \cdot 10^{-6}$  Torr) and at room temperature in IC-100 accelerator (NFL, JINR, Dubna). Low current ( $\sim 15$  nA) has been used to prevent the heating of the samples during the irradiation [14, 15]. X-ray analysis of TlFeS<sub>2</sub> monocrystals before and after radiation at room temperature was performed at D2 PHASER X-ray diffractometer.

The Xe<sup>+26</sup> ions with 167 MeV energy led to the formation of non-homogeneous radiation defects along the thickness of the samples. It has been determined the ionic loss energy  $(dE/dx)_{ion}$  and the number of radiation defects dpa (displacement per atom) along the depth of the path of Xe<sup>+26</sup> ions by using SRIM 2008.

According to the calculations, the Xe<sup>+26</sup> ions with the energy E=167 MeV are in the R=14.69 mkm running depth in the crystal. The crystalline properties of the samples irradiated at different doses have been investigated at the x-ray diffractometer. The parameters of a unit cell were calculated using the full-profile Rietveld analysis based on X-rays of the TlFeS<sub>2</sub> crystal before and after irradiation at different doses. The increased dose leads to the expansion of peaks and generates a background. Dose dependence of amorphous part of irradiated part by relative percentage has been defined by the method of full integral of a background area obtained from the spectra (Figure 1)

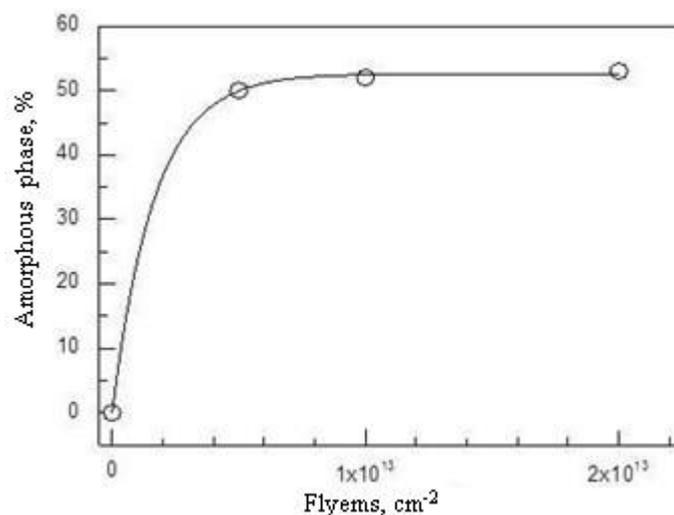


Fig. 1. Dose dependence of the amorphous part of the irradiated part by relative percentage

The obtained results show that crystals have a crystalline form of about 47%, without full amorphization in the irradiated layer. We think that the obtained x-ray images are reflections given by the residual crystalline structure and analysed in the C2/m symmetry group in the program. Crystalline parameters of  $\text{TlFeS}_2$  before irradiation were  $a = 11.63 \text{ \AA}$ ,  $b = 5.30 \text{ \AA}$ ,  $c = 6.82 \text{ \AA}$ ,  $\beta = 116.78$ ,  $V = 375.43 \text{ \AA}^3$ , but after the irradiation at  $2 \cdot 10^{13} \text{ cm}^{-2}$  radiation dose, they were  $a = 11.77 \text{ \AA}$ ,  $b = 5.31 \text{ \AA}$ ,  $c = 7.08 \text{ \AA}$ ,  $\beta = 118.71$ ,  $V = 388.07 \text{ \AA}^3$ .

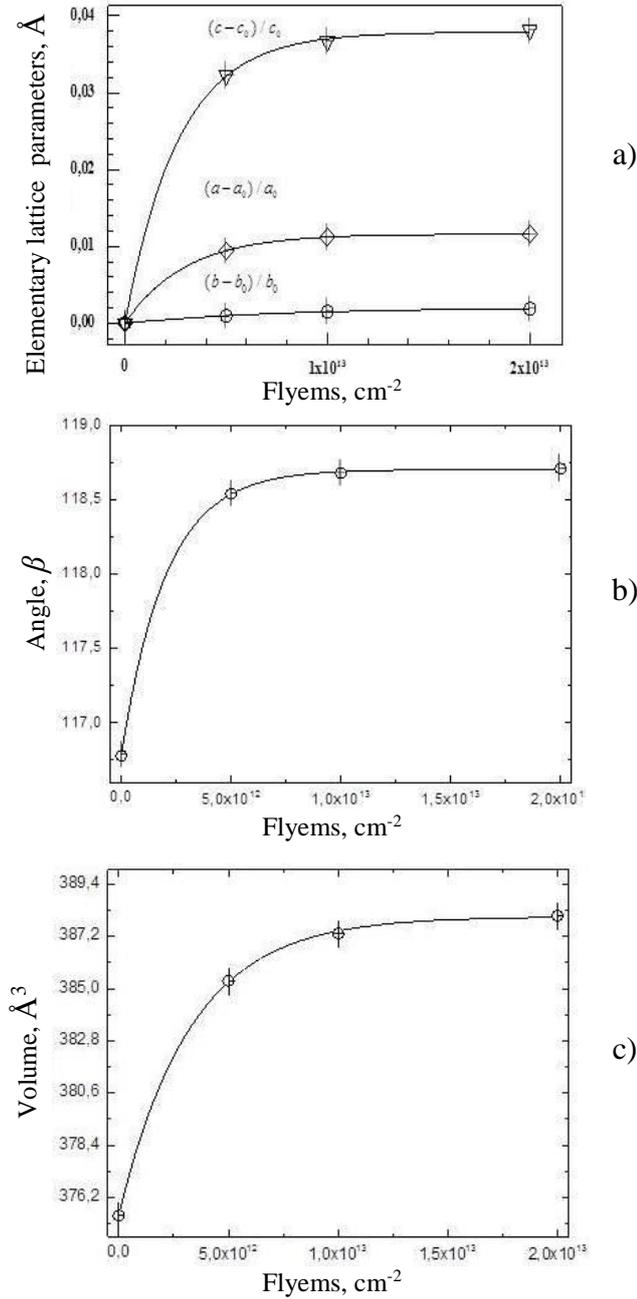


Fig. 2. a) Flyems dependence of relative change of unit cell parameters of  $\text{TlFeS}_2$  crystals, b) Flyems dependence of monoclinic angle in  $\text{TlFeS}_2$  crystals, c) Flyems dependence of volume of elementary lattice of  $\text{TlFeS}_2$  crystals.

The dependency curves of the relative change of the unit cell parameters and the monoclinic angle of TlFeS<sub>2</sub> crystals on radiation dose have been established (Figure 2 a, b, c). It seems from the curves that the crystallographic parameters increase by the dose growth and are stabilized after  $1 \cdot 10^{13} \text{cm}^{-2}$ . We believe that the subsequent increase after “critical” dose (approximately  $0.32 \sim 10^{13} \text{ ion/cm}^{-2}$ ) leads to the destabilization, destruction and structural change in crystalline cell and it is stabilized after  $1 \times 10^{13} \text{ ion/cm}^2$ , i.e., the speed of change is weakening, this limit is the limit of the values of crystallographic parameters [12, 13].

The surface of the samples irradiated with heavy Xe<sup>+26</sup> ions has also been studied. The investigation of surface morphology before and after irradiation was performed on SOLVER-NEXT atom-force microscope. Investigation of surface morphology before and after irradiation was performed on SOLVER-NEXT atom-force microscope. SOLVER-NEXT is a generic multifunctional probe microscope, with highly automated digital operations allowing the surface process to be studied by modern methods and in nano sizes. The atomic force microscopy method is one of the most sensitive methods and is able to obtain accurate information on the surface. The AFM’s working principle is based on the Van der Waals forces [16, 17].

Crystals are split into parts as separate layers for the purpose of obtaining an atomic scale pure surface, before the irradiation and the placement on the moving table of the atomic-force microscope. Depending on the power of radiation, the variety of regularity on the surfaces is shown in Figure 3.

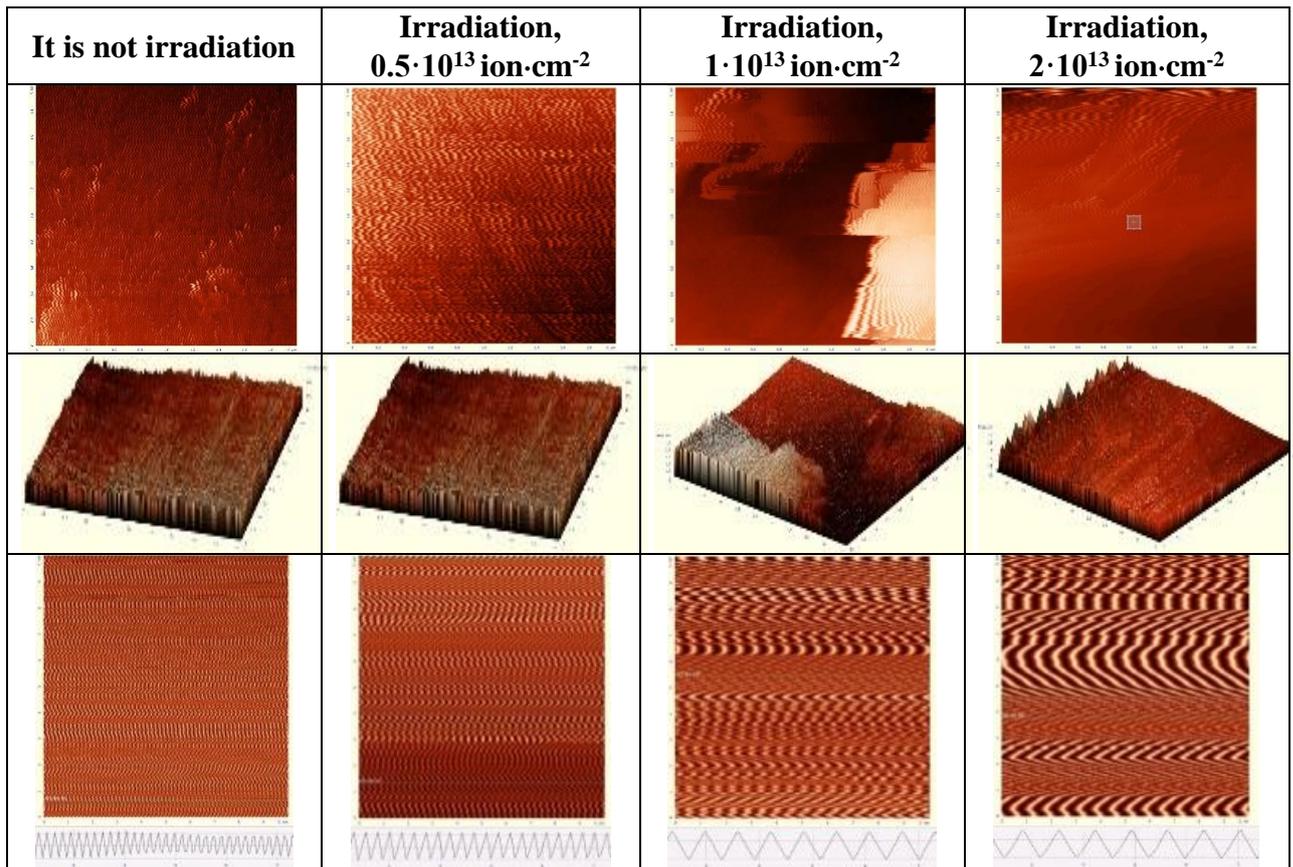


Fig. 3. 2D and 3D images before and after irradiation, variety of periodicity on the surfaces.

The images show that as the radiation dose increases, the peaks of the relief of the nanoscale surface decrease.  $\text{Xe}^{+26}$  ions increase the energy potential of the surface atoms, and many collisions increase the distance between the surface atoms, resulting in a decrease in periodicity in the nanoscale.

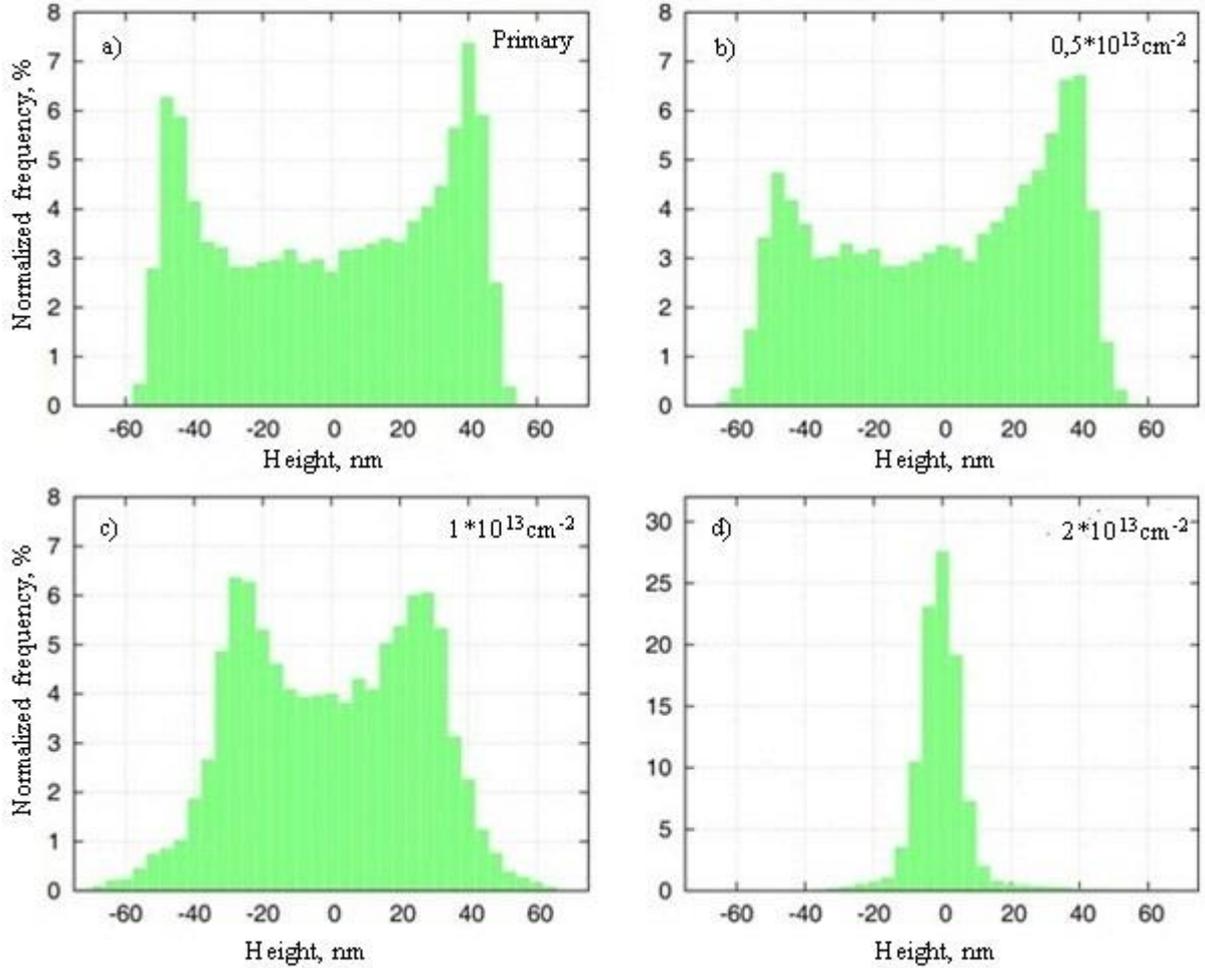


Fig. 4. Histograms of quantitative dependencies of the surface.

According to quantitative dependencies histograms of the surface obtained from atomic force microscopy (Figure 4), there is observed a change in the split periodicity structure of the surface, maximal value  $Z_{ij}$ , average square roughness  $S_q = \sqrt{\frac{1}{N_x N_y} \sum_{j=1}^{N_y} \sum_{i=1}^{N_x} Z_{ij}^2}$ , asymmetry

coefficient  $S_{sk} = \frac{1}{S_q^3 N_x N_y} \sum_{j=1}^{N_y} \sum_{i=1}^{N_x} Z_{ij}^3$ , concavity coefficient characterizing the sharpness of the

peaks  $S_{ka} = \frac{1}{S_q^4 N_x N_y} \sum_{j=1}^{N_y} \sum_{i=1}^{N_x} Z_{ij}^4$ . Dose dependence curves of these parameters characterizing the surface are shown in Figure 5.

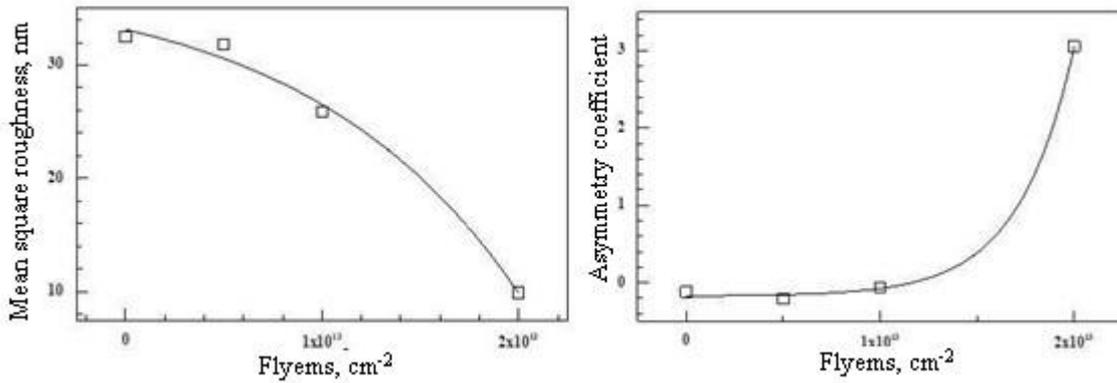


Fig. 5. Dose dependence curves of the parameters characterizing the surface

It is clear from histograms that as the radiation dose increases, the difference of depth and height of the surfaces  $\Delta Z$  covers smaller area from the zeroth plane of the surface, i.e., the surface roughness decreases and it becomes smoother. The histograms of the non-irradiated samples and irradiated at the  $0.5 \cdot 10^{13}$  ion/cm<sup>2</sup> dose did not change practically, i.e. the asymmetry and concavity coefficients are almost at close values. Asymmetric coefficient approaches zero from a negative value with subsequent increase in dose ( $1 \cdot 10^{13}$  ion/cm<sup>2</sup>) and the roughness decreases. The peak in the form of Gaussian are formed in the last value of the dose  $2 \cdot 10^{13}$  ion/cm<sup>2</sup>, then the asymmetry coefficient reaches a positive value and the surface becomes “smoother”.

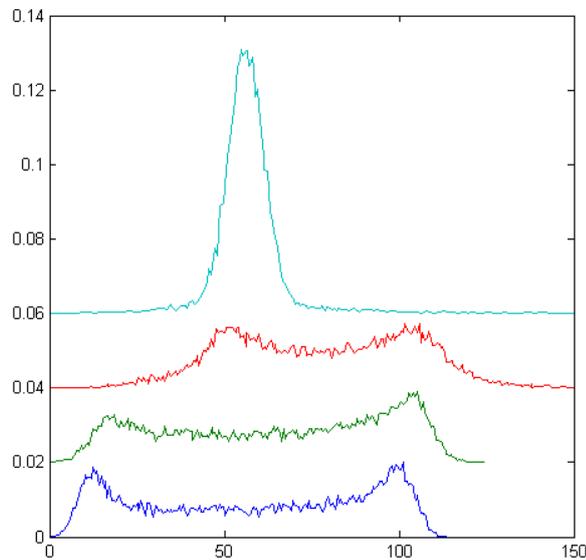


Fig. 6. The peak in the form of Gaussian at last value of dose  $2 \cdot 10^{13}$  ion/cm<sup>2</sup> in the histogram and parameters after analysis.

Figure 6 presents one-dimensional characteristic of the quantitative dependence histograms of the surface. The form of the Gaussian-shaped peak obtained at last dose seems clearly. As the dose increases, the double peaks get closer, i.e., the diminution in the difference between the convexity and concavity is observed and at last, the double peaks are replaced by a Gaussian-shaped peak.

### 3. Result

1. Elementary lattice parameters have been calculated before and after irradiation, radiation dose dependencies of crystallographic parameters were established. It has been determined that by the increase of the dose, the lattice parameters, the crystal lattice volume increase exponentially and are stabilized after the dose of  $1.0 \cdot 10^{13}$  ion /  $\text{cm}^{-2}$ .
2. The nanoscale morphology of the surface of  $\text{TlFeS}_2$  crystals before and after irradiation has been studied and it has been clarified that as the radiation dose increases, the number of peaks of periodicity of the atomic clusters of nanoscale surface decreases exponentially.

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## ЭФФЕКТЫ РАДИАЦИИ, СОЗДАННЫЕ С ИЗЛУЧЕНИЕМ ИОНАМИ В КРИСТАЛЛЕ $TlFeS_2$

**Р.Н. Мехтиева**

**Резюме:** В данной работе исследованы радиационная стойкость и формирование радиационных дефектов цепных полупроводниковых антиферромагнитных монокристаллов  $TlFeS_2$  облученных с тяжелыми ионами при различных дозах. Изучено влияние облучения тяжелых ионов ксенона на структуру облученного слоя после облучения, и было показано, что с увеличением дозы облучения число максимальной периодичности нано размерных поверхностных атомных кластеров экспоненциально уменьшается.

**Ключевые слова:** облучения ионами, имплантация, радиационные дефекты, поверхностная морфология

## İONLARLA ŞÜALANMANIN $TlFeS_2$ KRİSTALINDA YARATDIĞI RADİASİYA EFFEKTLERİ

**R.N. Mehdiyeva**

**Xülasə:** Bu işdə ağır ionlarla müxtəlif dozalarda şüalandırılmış zəncirvari yarımkeçirici antiferromaqnit  $TlFeS_2$  monokristalının radiasiyaya davamlılığı və radiasiya qüsurlarının formalaşmasına baxılmışdır. Şüalanmadan sonra şüalanmış təbəqənin struktur quruluşuna ağır ksenon ionları ilə şüalanmanın təsiri tədqiq edilmiş və göstərilmişdir ki, şüalanma dozası artdıqca nanoölçülü səthin atom klasterlərinin periodikliyinə maksimumlarının sayı eksponensial olaraq azalır.

**Açar sözlər:** ionlarla şüalanma, implantasiya, radiasiya defektləri, səth morfologiyası